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INITIATION MECHANISMS OF SOLID ROCKET
PROPELLANT DETONATION

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IIT Research Institute

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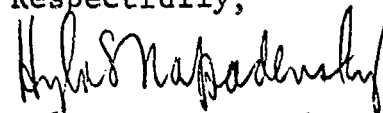
FOREWORD

This interim report summarizes the research that was conducted during the period 1 April 1971 through 31 March 1972. The work was sponsored by the Air Force Office of Scientific Research (AFOSR), Office of Aerospace Research, United States Air Force, under Contract F44620-71-C-0060.

Technical Supervisor for this program period was Lt.Col. R. W. Haffner, Energetics Division, Air Force Office of Scientific Research.

The IIT Research Institute (IITRI) personnel who have contributed to this research are C. A. Kot and H. S. Napadensky.

Respectfully,



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ABSTRACT

The mechanisms which may lead to detonation initiation in solid rocket propellants due to accidentally applied low amplitude stimuli are studied. In particular, the effects of low speed impact are studied. A two-dimensional Lagrangian computer code is used to study the detailed hydrodynamic (or elastic-plastic) and thermodynamic behavior of propellant materials under impact conditions. It was found that only moderate temperature increases ($\sim 200^{\circ}\text{C}$) are generated in unconfined impact of a cylindrical material billet upon a rigid surface. When a second boundary is introduced, i.e., the material is at rest on a rigid base and is impacted by a rigid plate, the temperatures developed under certain conditions exceed the values achieved in unconfined impact by more than a factor of two. This is due to the multiple shock reflections taking place at the rigid boundaries. Based on many numerical experiments both for unconfined and plate impact, and using material cylinders of various aspect ratios, it is concluded that the primary mechanism responsible for the temperature rise is the adiabatic compression of the material. This implies that compressibility and hydrodynamic wave motion are dominant in producing localized energy concentrations and subsequently high temperature rises. The energy due to distortion or friction contributes little to the total temperature increase.

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1. INTRODUCTION

The objective of this program is to obtain an understanding of the phenomena which may lead to the initiation of detonation in solid rocket propellants. The interest is limited to stimuli which are representative of typical accident conditions, i.e., stimuli of moderate amplitude.

The existing detonation theories describe, reasonably well, the steady-state detonation of propellants and explosives by strong shock waves. However, detonation of propellants and explosives can occur under low amplitude shocks and by impact at speeds and pressures that are well below those predicted by hydrodynamic theory of detonation. Equally important as high order detonation is the class of chemical decompositions referred to as subdetonation reactions. Such reactions occur when the stimulus is not sufficient to cause high order detonation but is sufficient to cause disturbances with intensity levels ranging from mild burning to low order detonation. Subdetonation reactions occur at relatively low pressures; hence, they are of interest in determining the potential hazards of propellants to common accidental stimuli such as impact or mechanical action.

Large deformations characterize the mechanical response of solid propellant materials prior to initiation in realistic accidental impact situations and in low velocity unconfined impact experiments. An understanding of material flow and energy conversion processes in dynamic compression is required to determine the mechanisms responsible for propellant ignition in low speed impact.

The current study is a continuation of work done under an earlier contract (F44-620-67-C0081, Reference 1). This project includes both experimental and theoretical efforts. The experimental work involved flyer plate impact experiments for the determination of deformation modes, impact speeds required for initiation, and intensity of reaction. Instrumentation consisted primarily of high speed photographic coverage. The gross overall

phenomena can be readily observed and data on initiation thresholds collected in such experiments. However, it is not possible to gain insight into the detailed mechanisms contributing to the initiation of the propellant material under impact conditions. Therefore theoretical and numerical modeling of the propellant impact problem was undertaken. In contrast to experimental work the numerical effort permits a detailed investigation of the phenomena taking place during impact. This in turn leads to a better understanding of the parameters which may play an important role in the initiation of propellants. Theoretical calculations can also enhance the interpretation of experimental results, while the latter may be used to check the computations. During the most recent period emphasis has been placed on the computational modeling of impact phenomena.

2. COMPUTER PROGRAM DEVELOPMENT

The primary tool employed in the modeling of propellant impact is a two-dimensional Lagrangian computer code developed specifically for this purpose. Both plane two-dimensional geometries and axisymmetric cylindrical shapes may be modeled. Material behavior can be either hydrodynamic or elastic-plastic. The latter is particularly important for low velocity impacts where stress levels are not sufficiently great to permit a hydrodynamic idealization of the material. The code is based on well established numerical techniques (Reference 2) and has been previously described in some detail (Reference 3). Originally the computer program was restricted to the modeling of unconfined impact in which a cylindrical billet of material impacts a rigid surface which is perpendicular to the cylinder's axis. The deformation of the impacted material, the wave propagation and the flow fields were analyzed in these early calculations. Since temperature is a good measure of the likelihood of initiation occurrence in the propellant, the capability of computing this variable was added to the computer program at least for one form of the equation of state (see Reference 3). Also the treatment of surface friction at the rigid surface was incorporated into the code. Other boundary conditions that may be simulated at this surface are free-slip or no-slip conditions.

More recently the capability of simulating the impact of a flyer plate on a billet of material which in turn rests on a rigid surface has been added to the code. This configuration is typical of impact sensitivity tests used both for explosives and propellants. To aid in the interpretation of the computational results, a capability for graphical display of the deformed propellant billet has been developed. Basically the generated plots represent the current location of the computational grid.

A homogeneous material behavior has been assumed for all of the computations performed. Both propellants and explosives have been considered. The latter provide a basis for comparison since extensive information exists regarding their properties and equation of state data. A caloric form of the equation of state, relating pressure, density, and specific internal energy, is required to perform hydrodynamic or elastic-plastic computations. However, in order to study possible initiation mechanisms an estimate of the temperature field must be made. This in turn requires a thermal equation of state which relates temperature to the other thermodynamic variables. While caloric equations of state may be derived from rather simple experimental data, more detailed information is required to describe the thermal behavior. These data are usually not available for complex propellant materials. Since the objective is to estimate the temperature field in a homogeneous material under low speed impact conditions prior to actual chemical reaction, explosives, and in particular TNT, for which equation of state data are more readily available, has been extensively used in the computations. It is felt that the results thus obtained are at least qualitatively representative of the mechanisms contributing to a significant temperature rise in any homogeneous material.

3. RESULTS, SUMMARY, AND DISCUSSION

Many of the results obtained from the computational efforts of this program have been previously reported (see References 1, 3, and 4). Regarding the main objective of this study, i.e., the investigation of possible initiation mechanisms during impact, the temperature rise in the material has been used as a measure and criterion for the likelihood of initiation occurrence.

During unconfined impact the temperatures throughout the material were generally quite moderate. Material differences produced noticeable but small differences in the computed temperature fields. Hydrodynamic modeling of the materials resulted in somewhat higher temperatures than when material strength (elastic-plastic behavior) was taken into account. Similarly the computations for propellant materials such as EJC and PBAN produced higher temperatures than the calculations for TNT. However all of these temperatures were found in the neighborhood of 200°C and are probably too low to produce initiation or significant chemical reactions within the materials. No enhancement of the maximum material temperatures during impact was obtained by the inclusion of surface friction in the computations. It is possible that higher temperatures may occur directly at the surface but cannot be resolved in the computations. Even for very fine grids no significant temperature increases due to friction could be ascertained.

Larger temperature increases were calculated only when impact under semiconfined conditions was considered. In these computations it was assumed that a billet of material is impacted by a rigid plate while resting on a rigid surface. This is a geometry typical of the flyer plate sensitivity experiments. The same size billet as for the unconfined impact (5 cm radius and 5 cm height) was assumed. The plate impact speed was also the same as for the billet impact (21 cm/msec). A steel flyer plate of one inch

thickness was considered. Under these conditions a localized high temperature ($\sim 400^{\circ}\text{C}$) occurred for a short duration in the impacted material. Typical of the results obtained is the maximum temperature variation with time shown in Figure 1 as a solid line. A rapid initial temperature rise is followed by about 20 μsec of nearly constant maximum temperature, as the shock caused by the plate impact traverses the billet in the downward direction. Upon shock reflection at the bottom rigid surface the temperature takes a rapid jump to its maximum value of nearly 400°C . Due to the absence of such a reflecting surface in unconfined impact, the temperature does not experience a second rapid increase and the maximum temperature obtained is much lower (see Reference 1). After reaching this peak value the maximum temperature decreases rapidly as the rarefaction waves originating from the lateral free surface relieve the pressure in the material. During the temperature increase the region through which the maximum temperature prevails in the radial direction shrinks continuously as the rarefaction waves progress toward the centerline of the cylindrical billet. This is shown in Figure 2 along with typical temperature profiles. In the radial profile there is a constant temperature region in the vicinity of the centerline and then a gradual temperature decrease toward the lateral surface of the cylinder. The axial profile exhibits a behavior typical for the passage of a shock wave, i.e., a rapid rise from ambient conditions to a maximum value followed by a gradual decay behind the shock front.

Based on these results it was concluded that the primary mechanism responsible for the temperature rise is the adiabatic compression of the material. This implies that the compressibility and hydrodynamic aspects of the material behavior are dominant in producing high temperatures and that the energy of distortion contributes little to the temperature rise. To test this conclusion additional computations were performed, again assuming a flyer plate impact but for a narrower cylinder (2.5 cm radius and 5.0 cm height).

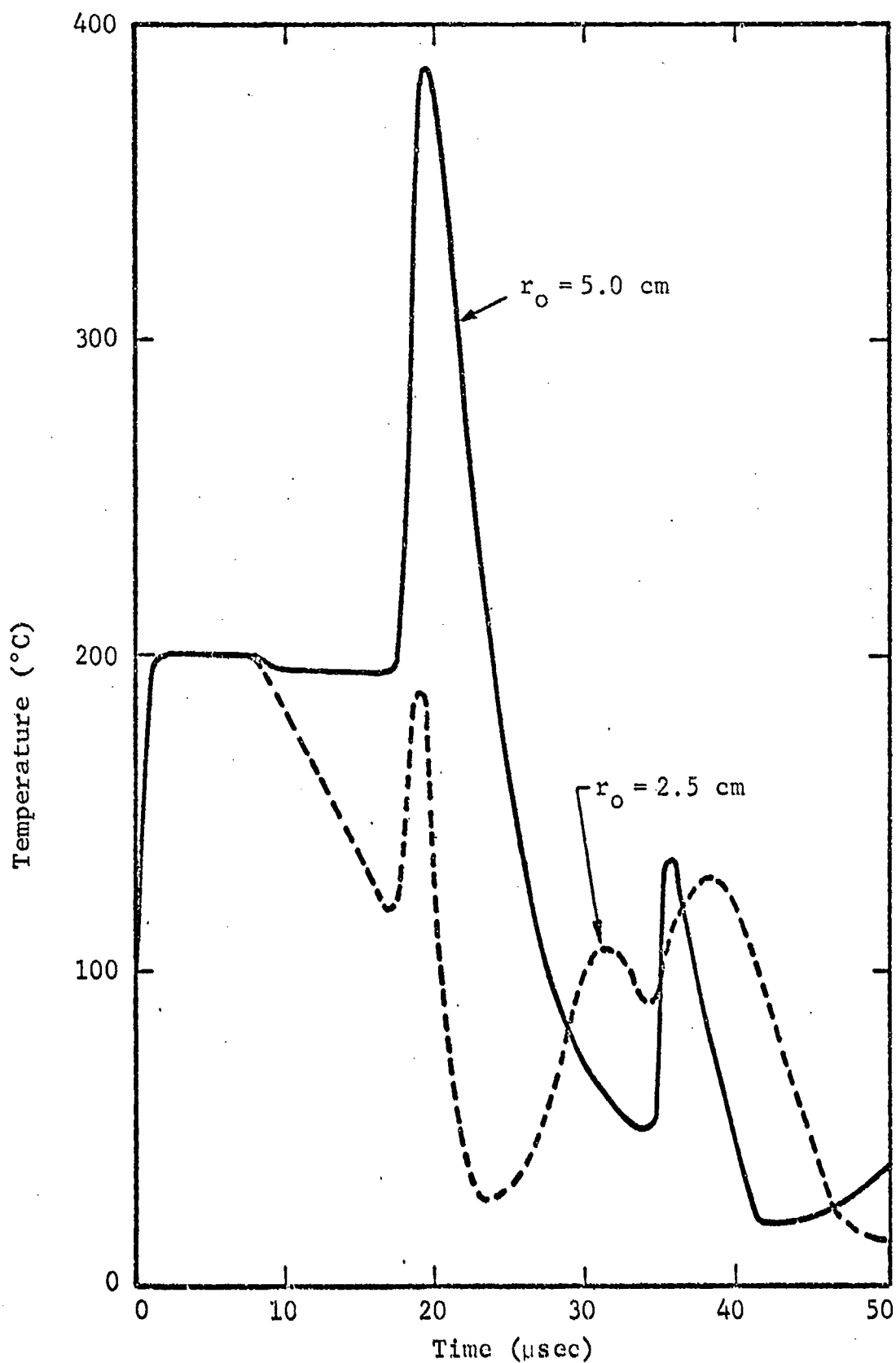
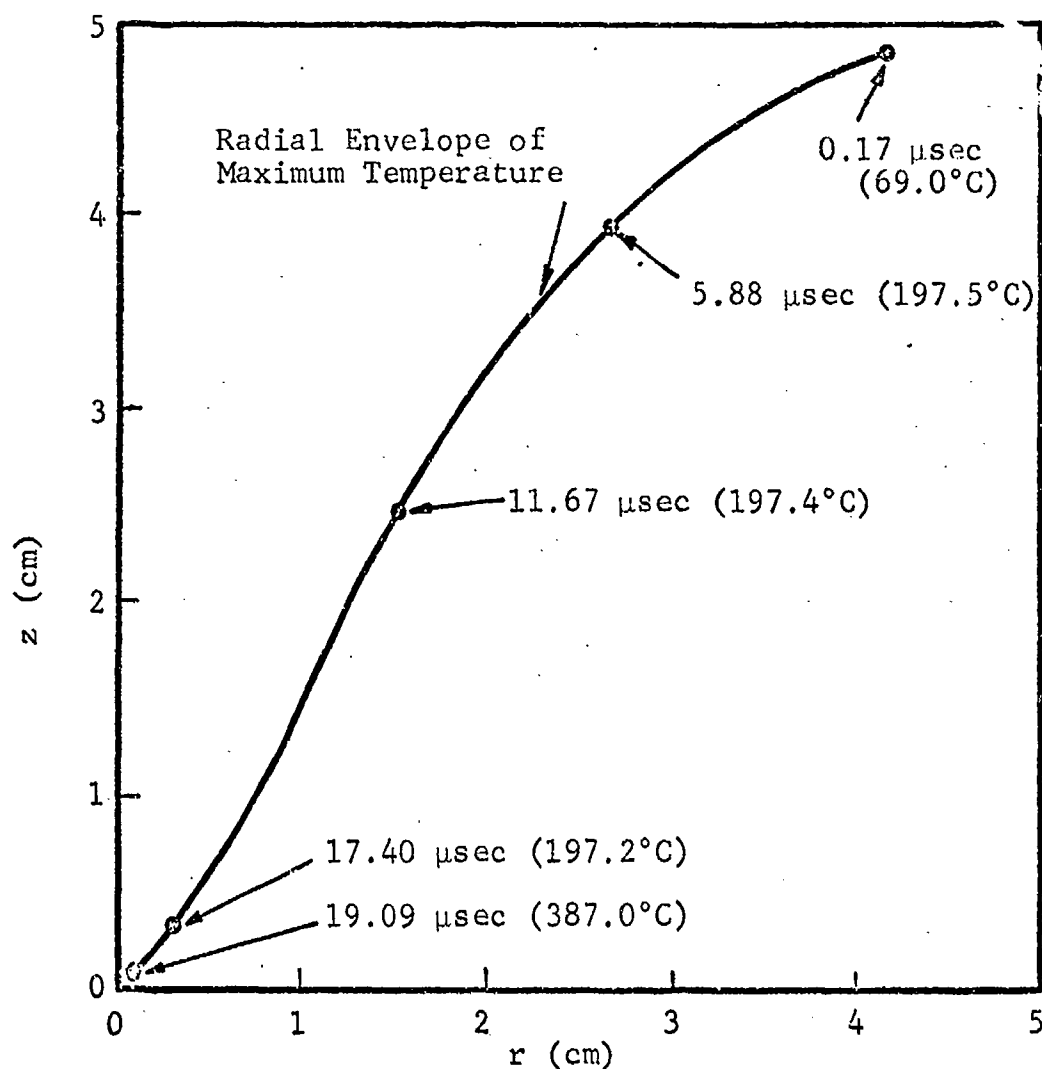
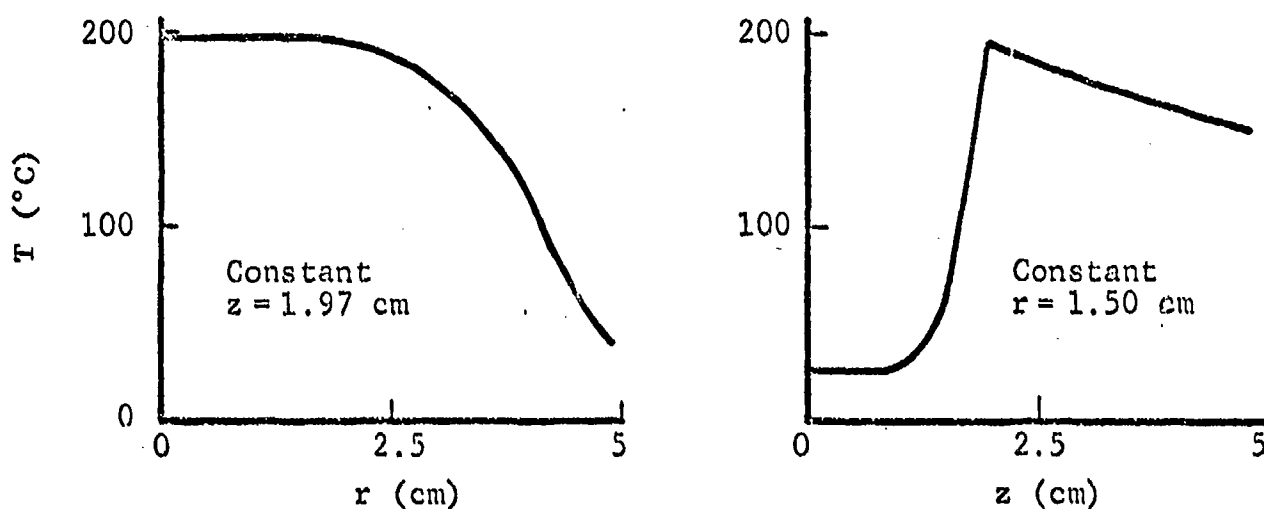


Figure 1 Maximum Temperature versus Time for TNT Elastic-Plastic, Free-Slip Boundary



Location of Maximum Temperature

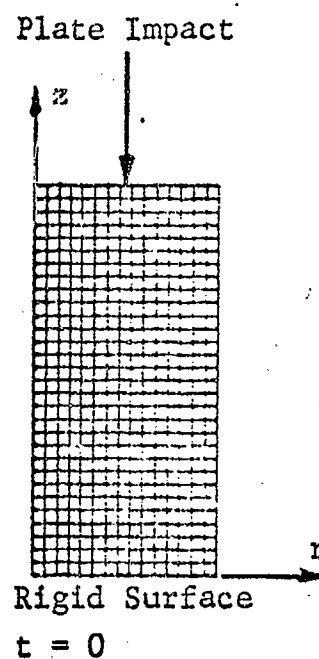
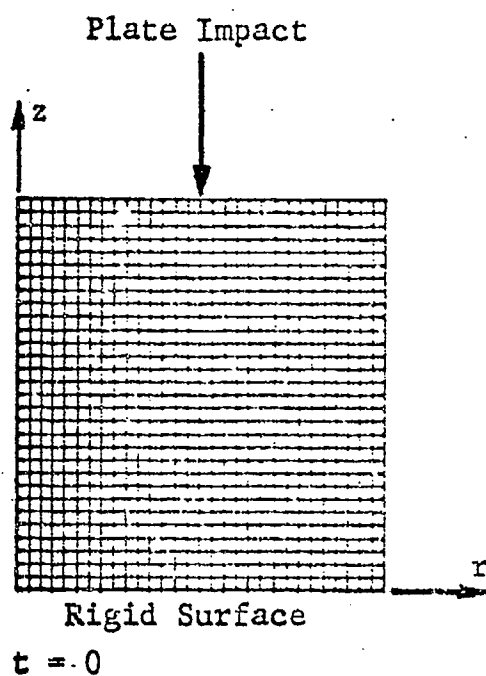


Temperature Profiles at Time $t = 11.67 \mu\text{sec}$

Figure 2 Spatial Variation of Temperature for TNT Elastic-Plastic, Free-Slip Boundary

The maximum temperatures as a function of time for these calculations are shown in Figure 1 as a dashed line. While the behavior is qualitatively similar to that of the wider cylinder, the second temperature peak due to shock reflection is actually lower than the temperature behind the original shock. This is due to the fact that the rarefaction waves coming from the lateral surface had sufficient time in the narrow cylinder to penetrate to the centerline and thus lower the pressure behind the incident shock before reflection took place. This confirms our earlier conclusion that high temperatures in the material are produced by adiabatic compression. The deformation of the narrower cylinder is as great or greater than that experienced by the larger cylinder. This can be seen in Figure 3, which represents the mesh distortion of the cylinders at approximately equal times.

The computations modeling the flyer plate impact were carried out both for a free-slip and no-slip boundary condition at the bottom or anvil rigid surface. The resulting maximum temperatures were found to be virtually the same in both cases. This can be seen by comparing Figure 1 with Figure 4, where the latter presents the maximum temperature as a function of time for the no-slip case. The deformation has only insignificant influence on the temperature and adiabatic compression is the dominant effect. In Figure 5 a typical variation of pressure and density, at the location of the maximum temperature, is shown as a function of time. Also shown is the maximum temperature itself. We see that the pressure and density variations follow the variation of temperature exactly. The shown pressures and densities are the highest values encountered in the field. Hence the hydrodynamics behavior of the material regarding its temperature rise is again demonstrated.



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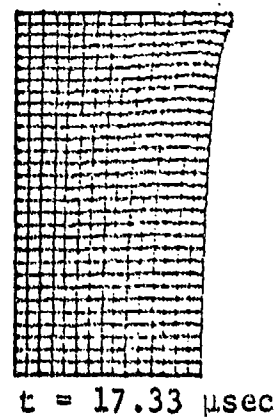
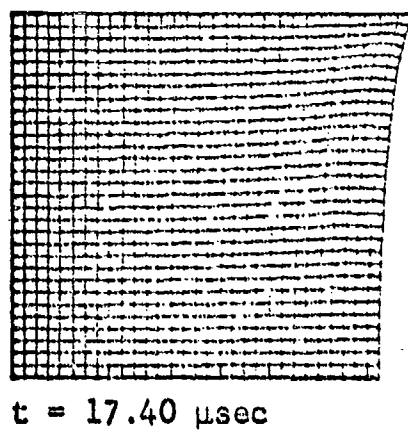
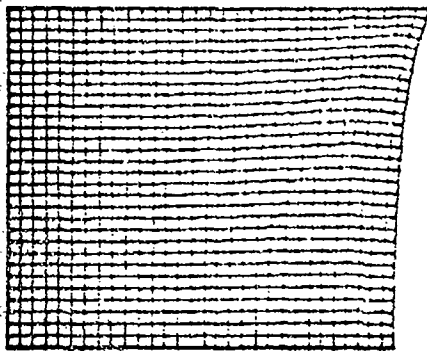
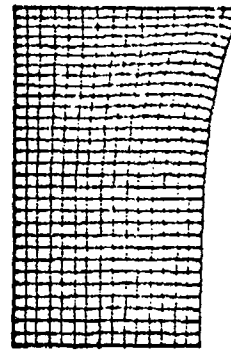


Figure 3a Comparison of TNT Billet Deformations,
Plate Impact $V_0 = 21 \text{ cm/msec}$

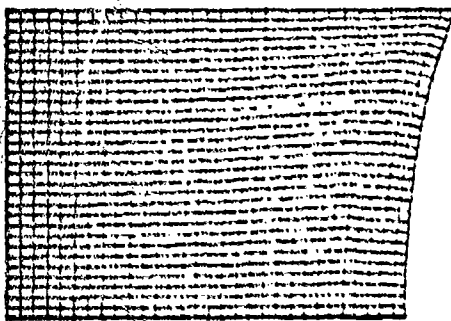


$t = 33.49 \mu\text{sec}$

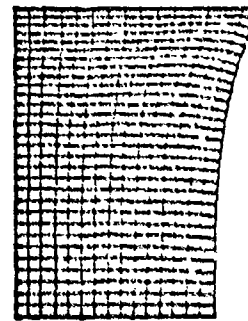


$t = 33.05 \mu\text{sec}$

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$t = 54.36 \mu\text{sec}$



$t = 52.90 \mu\text{sec}$

Figure 3b Comparison of TNT Billet Deformations,
Plate Impact $V_0 = 21 \text{ cm/msec}$

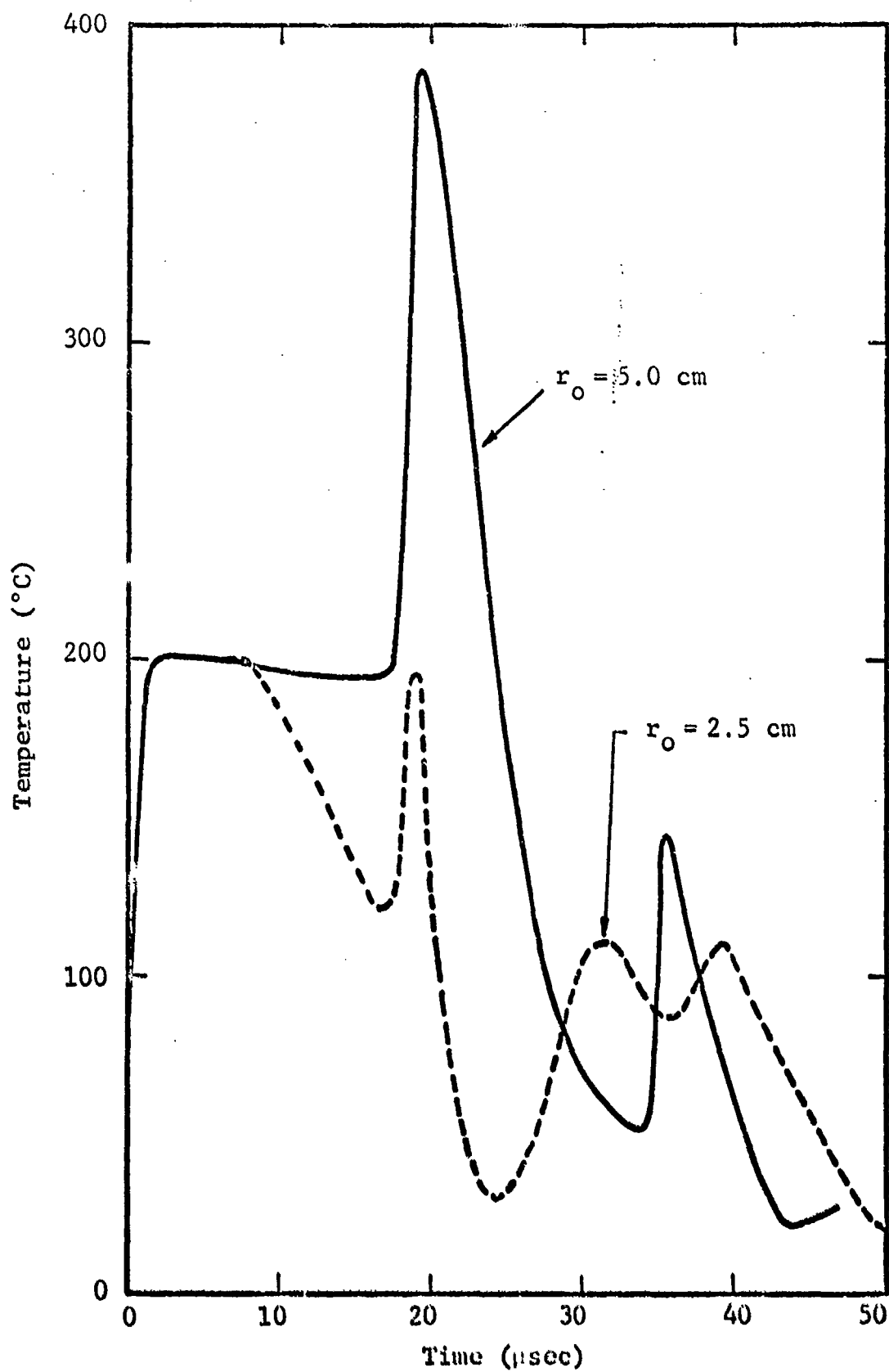


Figure 4 Maximum Temperature versus Time for TNT Elastic-Plastic, No-Slip Boundary

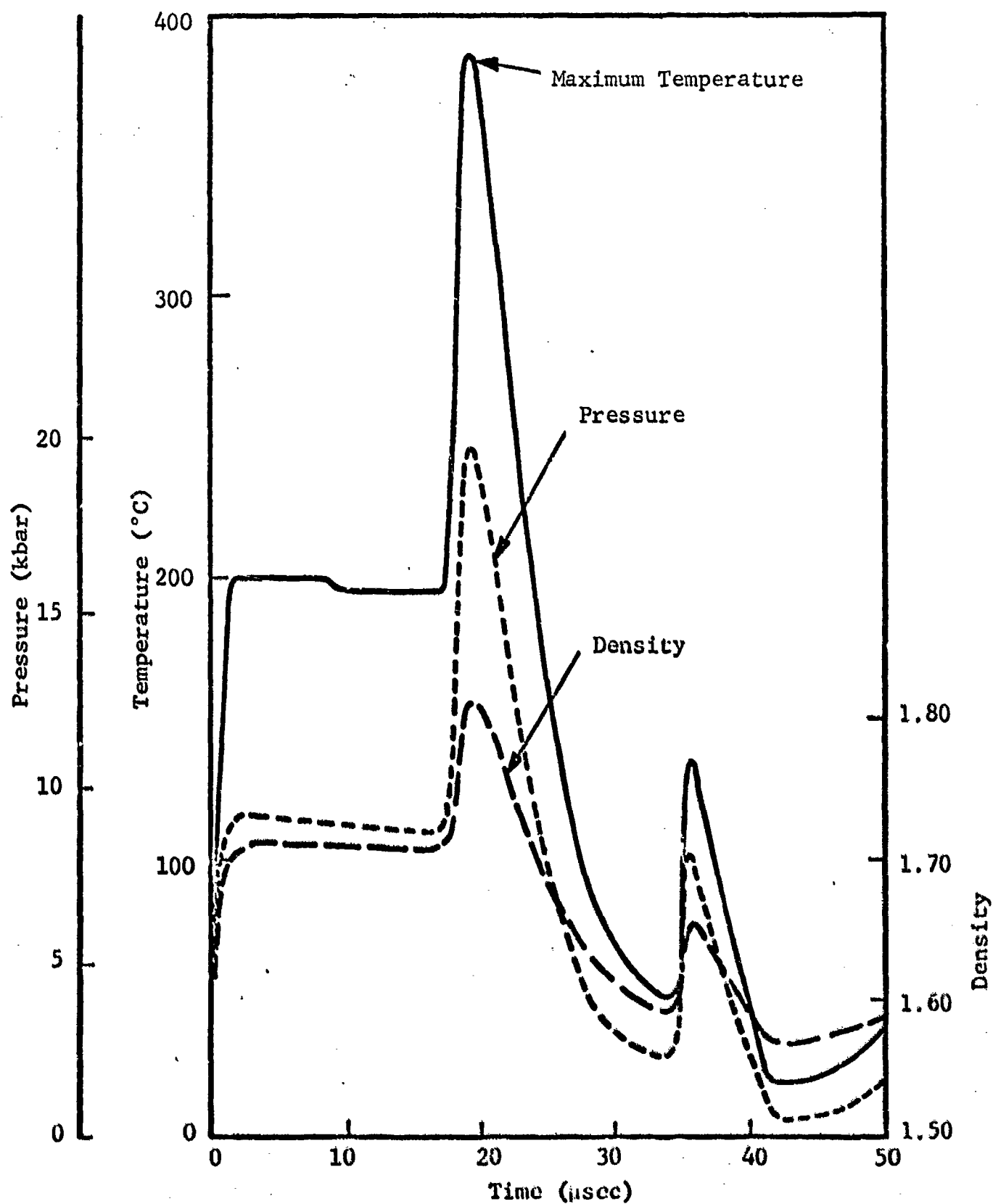


Figure 5 Variation of Maximum Temperature, Pressure, and Density for TNT, Elastic-Plastic, Free-Slip Boundary

The highest temperatures in the material are limited to a small spatial region (approximately a sphere of 0.08 cm radius) and occur only for very short durations (a few microseconds). However, other investigators have shown (Reference 5), that at a temperature around 400°C initiation sources or hot-spots of these dimensions and durations are sufficient to cause initiation. Thus our calculations indicate that initiation may take place in a completely homogeneous material due to purely hydrodynamic mechanisms of energy concentration. This focusing of energy depends on the geometry and details of the applied load. While the presence of inclusions such as voids, bubbles or impurities may enhance the chance of initiation, they are not a necessary condition for initiation.

To investigate the significance of inclusions or material inhomogeneities the presence of a small gas bubble can be modeled numerically. Similarly the influence of further material confinement by bulkheads or casing can be numerically studied. These considerations require the modification of the computer code to allow the treatment of multiple materials. Such modifications are now in progress. Effort is also being devoted to the modeling of heat evolution during impact, the development of initiation criteria, and the subsequent treatment of reaction propagation.

4. SIGNIFICANT PROGRAM INTERACTIONS AND PUBLICATIONS

The theoretical and experimental techniques developed in the course of this program have found broad applications in other DOD projects. In particular during the past year the numerical methods were applied to the study of hydrodynamic phenomena associated with the performance of fuel-air explosive munitions (Contract F08635-71-C-0040). Similarly the experience gained has been found valuable in the treatment of underwater explosion phenomena. The experimental know-how acquired was used in evaluating the sensitivity of new propellant formulations (Contract F04611-71-C-0042). During the reporting period of 1 April 1971 to 31 March 1972 IITRI personnel presented talks and publications which are based on the work of this program or related endeavors.

Kot, C. A., "Intense Underwater Explosions", Third International Colloquium on Gasdynamics of Explosions and Reactive Systems, Marseille, France, 12-17 September 1971.
(Accepted for publication in *Astronautica Acta*)

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Napadensky, H. S., "Hazards to Explosive and Propellant Systems", 12th Annual Symposium - Behavior of Explosives in Engineering Design, Albuquerque, New Mexico, 2-3 March 1972.

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